Conda

Conda is a free software package and environment manager used primarily for scientific Python and R packages, but also supports other languages such as C, C++, FORTRAN, Java, Scale, Ruby and Lua.

Use Conda in TeideHPC

Once we have connected to the login nodes, we will have to load the `miniconda` module to start using *conda*:

```
module load Miniconda2/4.7.10
```

Once the software is loaded, we can, for example, see the version information of *conda*:

```
conda info
    active environment : None
      user config file : /home/vjuidias/.condarc
 populated config files : /home/vjuidias/.condarc
       conda version : 4.7.10
   conda-build version : not installed
      python version : 2.7.16.final.0
    virtual packages :
    base environment : /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10  (read only)
        channel URLs : https://conda.anaconda.org/conda-forge/linux-64
                       https://conda.anaconda.org/conda-forge/noarch
                       https://conda.anaconda.org/bioconda/linux-64
                       https://conda.anaconda.org/bioconda/noarch
                       https://repo.anaconda.com/pkgs/main/linux-64
                       https://repo.anaconda.com/pkgs/main/noarch
                       https://repo.anaconda.com/pkgs/r/linux-64
                       https://repo.anaconda.com/pkgs/r/noarch
                       https://conda.anaconda.org/r/linux-64
                       https://conda.anaconda.org/r/noarch
       package cache : /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/pkgs
                       /home/vjuidias/.conda/pkgs
    envs directories : /home/vjuidias/.conda/envs
                       /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/envs
            platform : linux-64
          user-agent : conda/4.7.10 requests/2.22.0 CPython/2.7.16 Linux/3.10.0-327.el7.x86_64 centos/
7.2.1511 glibc/2.17
               UID:GID : 1136:1136
            netrc file : None
          offline mode : False
```

Now we have to initialise the shell to use Conda. **This step is only necessary the first time**. If we don't do it, when using conda, we will get this message:

```
CommandNotFoundError: Your shell has not been properly configured to use 'conda activate'.
To initialize your shell, run

    $ conda init <SHELL_NAME>

Currently supported shells are:
  - bash
  - fish
  - tcsh
  - xonsh
  - zsh
  - powershell

See 'conda init --help' for more information and options.

IMPORTANT: You may need to close and restart your shell after running 'conda init'.
```

So, what we have to do is:

```
conda init bash
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/condabin/conda
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/bin/conda
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/bin/conda-env
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/bin/activate
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/bin/deactivate
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/etc/profile.d/conda.sh
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/etc/fish/conf.d/conda.fish
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/shell/condabin/Conda.psm1
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/shell/condabin/conda-hook.ps1
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/lib/python2.7/site-packages/xontrib/
conda.xsh
no change     /opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/etc/profile.d/conda.csh
modified      /home/vjuidias/.bashrc

==> For changes to take effect, close and re-open your current shell. <==
```

By doing this, we have modified the shell, in this case, our bash. We have added the following lines to the file `~/.bashrc`:

```
# >>> conda initialize >>>
# !! Contents within this block are managed by 'conda init' !!
__conda_setup="$('/opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/bin/conda' 'shell.bash' 'hook' 2> /
dev/null)"
if [ $? -eq 0 ]; then
    eval "$__conda_setup"
else
    if [ -f "/opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/etc/profile.d/conda.sh" ]; then
        . "/opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/etc/profile.d/conda.sh"
    else
        export PATH="/opt/envhpc/slurm19/rhel7/Miniconda2/4.7.10/bin:$PATH"
    fi
fi
```

```
unset __conda_setup
# <<< conda initialize <<<
```

For the changes to take effect, we have to log out of the login node and log back in. Once this is done, we will be able to use conda, install packages and create environments.

Create an environment in /data

By default, Conda will create an environment and install all software on the user's `/home` partition. This storage is limited in size, so we should configure the environments and install the software in the `/data` partition. To do this, we simply need to specify the path to Conda:

```
conda create -p data/myenvironment mysoftware

Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

 environment location: /data/vjuidias/myenvironment
 ...
```

And we activate it in the same way, specifying the route:

```
conda activate /data/vjuidias/myenvironment
```